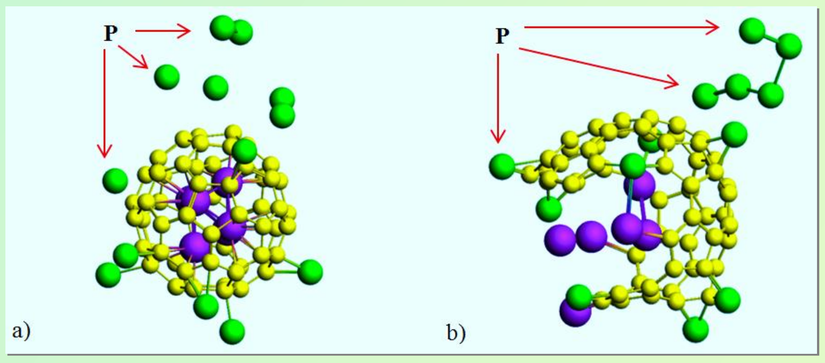
SELF-STABILITY OF $C_{60}@C_{180}$ DOUBLE LAYER NANOCAPSULES

DR. ALEJANDRO VALDERRAMA ZALDIVAR[1,2], M. EN C. RAÚL GÓMEZ[1], DRA. VIVIANNE MARQUINA FÁBREGA[1,2]

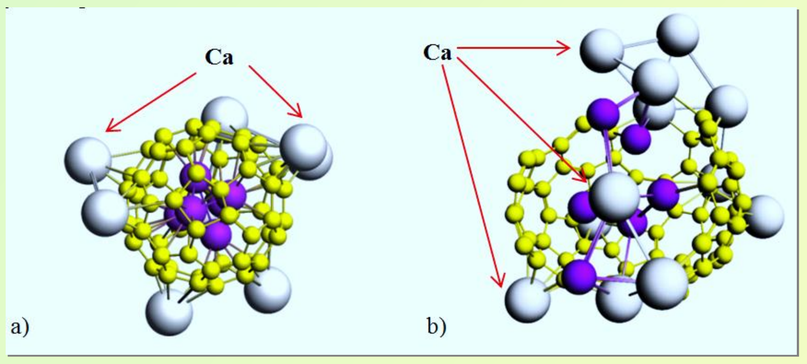
[1] FACULTAD DE CIENCIAS, UNIVERSIDAD NACIONAL AUTÓNOMA DE MÉXICO, APARTADO POSTAL 20-364, C.P. 01000, CDMX.

[2] POSGRADO EN CIENCIA E INGENIERÍA DE MATERIALES, UNIVERSIDAD NACIONAL AUTÓNOMA DE MÉXICO, APARTADO POSTAL 20-364, C.P. 01000, CDMX.

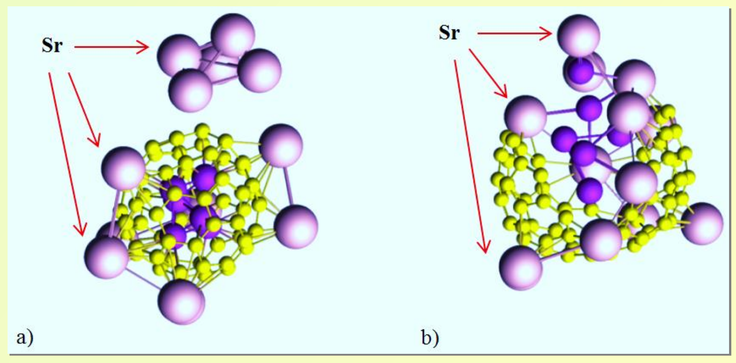
Supercomputing parallel processing Quantum Espresso code, and the Electronic Density Functional Theory (DFT), with the Perdew-Burke-Ernzerhof (PBE) exchange-correlation norm-conserving pseudo potentials is used to calculate the optimal configuration of the well-known fullerene C_{60} containing three radioactive iodine diatomic molecules ($3^{131}I_2$). In presence of calcium, phosphorus and strontium atoms, this system shows instability and when they are adsorbed, the fullerene disrupts releasing its content of radioactive iodine.



[Figure 1] DFT relaxation of the nanocapsule $3^{131}I_2@C_{60}$ surrounded by 13 ^{32}P atoms. a) In the first calculation cycles the adsorption of phosphorus on the surface is observed. b) After a few cycles of calculation fullerene breaks and releases its contents.

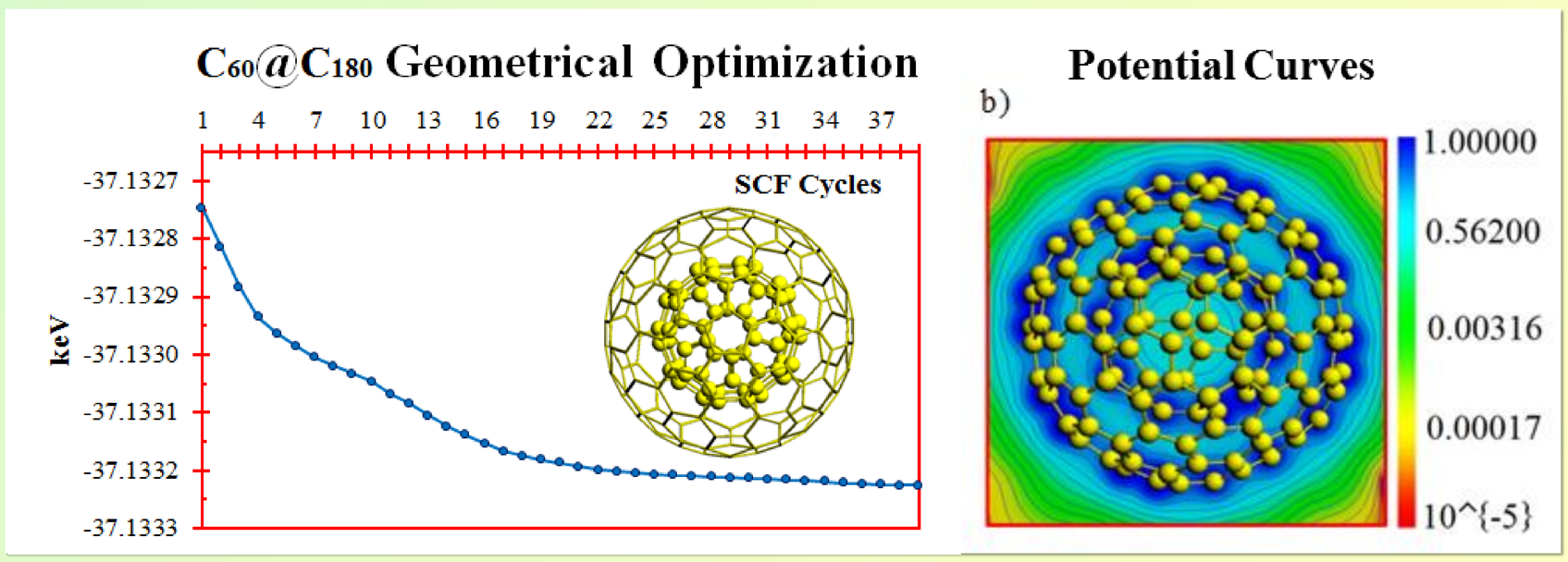


[Figure 2] DFT relaxation of $3^{131}I_2@C_{60}$ nanocapsule atoms surrounded by 13 Ca. a) In the first calculation cycles calcium adsorption is observed on the surface. b) The nanocapsule ends up breaking releasing iodine content.



[Figure 3] In this representation $3^{131}I_2@C_{60}$ nanocapsule is surrounded by 13 ^{89}Sr atoms atoms. a) Initially the adsorption of strontium is observed on the surface. b) When the relaxation evolve nanocapsule disrupts.

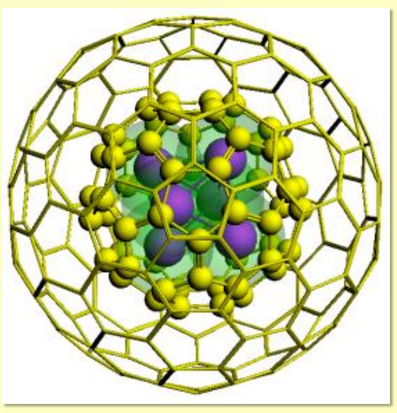
Thus, we performed the multi-layer fullerene simulation composed by the fullerene C_{60}, inside the buckyball C_{180}. We found that this system of two concentric carbon spheres has the energy **-37.133 keV** at the ground state.



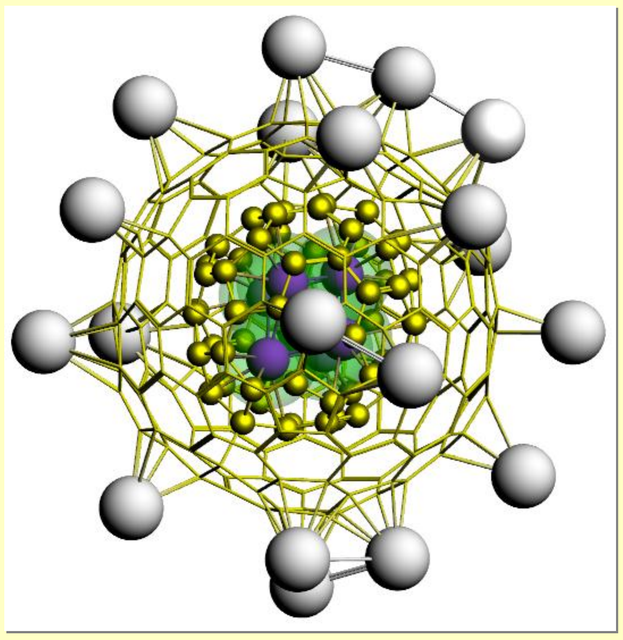
[Figure 4] a) The graph shows the convergence of the system to the ground state. In the representation the outer sphere C_{180} atoms of $C_{60}@C_{180}$ were removed to facilitate visualization of the whole. For this arrangement of two concentric fullerenes the total relaxation energy for the base state is **= - 37.133 keV.**

The system is strongly linked.

b) In this figure regions are also shown in dark blue regions of positive potential and clear blue practically neutral potential.



[Figure 5] This system can store, in the inner sphere C_{60}, the three diatomic molecules of radioactive iodine ($3^{131}I_2$), with an energy for the ground-state of **– 38.956 keV**.



[Figure 6] The multilayer nanocapsule can adsorb up to 20 calcium atoms on the outer sphere, C_{180}, surface with a total energy for the ground-state of -49.117 keV.

Conclusion: The system: $3^{131}I_2@C_{60}@C_{180}$ + 20Ca, is stable and constitutes a nanocapsule model with radioactive content capable to interact with other molecules with chemical calcium affinity, like crystalline calcium phosphate [$Ca_{10}(PO_4)_6(OH)_2$], as those occurring in the bones in the form of hydroxyapatite.

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